Solvent System Database for the Design and Prediction of Process Equilibrium

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Perhaps the most well known set of solvent and solute descriptors are the Kamlet-Taft parameters. These parameters provide numerical values for three important solvent and solute interactions; dipolarity-polarizability, hydrogen-bond donor ability, and hydrogen-bond acceptor ability. Historically, scales of these parameters have been established to allow for qualitative intercomparison of solvent and solute properties. These parameters can also be used quantitatively in modeling solution equilibrium in the form of a linear solvation energy relationship (LSER). A database that includes both pure solvent parameters and binary mixture parameters will be demonstrated. The database will provide predictive solvent selection capability using an LSER routine for a solution process that is input by the user. For example, the solubility of a compound in a series of solvents can be input and modeled as an LSER by the program using the parameters in the database. Based on the computed LSER, a solubility and the precision of the estimate can be predicted in a potential solvent or solvent system. The initial form of the database will include literature values for approximately 250 common organic solvents and the glycol ether solvents and glycol ether/ water solvent mixtures that we have recently measured.